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A SUMMARY OF THE ASSESSMENT OF FUEL BEHAVIOUR, FISSION PRODUCT RELEASE AND PRESSURE TUBE INTEGRITY FOLLOWING A POSTULATED LARGE LOSS-OF-COOLANT ACCIDENT

by

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A SUMMARY OF THE ASSESSMENT OF FUEL BEHAVIOUR, FISSION PRODUCT RELEASE AND PRESSURE TUBE INTEGRITY FOLLOWING A POSTULATED LARGE LOSS-OF-COOLANT ACCIDENT

A report prepared by V.J. Langman and K.R. Weaver of IDEA Research, Toronto, Canada, under contract U2SQ.87055-3-4033 to the Atomic Energy Control Board, Ottawa, Canada.

ABSTRACT

The Ontario Hydro analyses of fuel and pressure tube temperatures, fuel behaviour, fission product release and pressure tube integrity for large break loss-of-coolant accidents in Bruce A or Pickering A have been critically reviewed. The determinations of maximum fuel temperatures and fission product release are very uncertain, and pressure tube integrity cannot be assured where low steam flows are predicted to persist for times on the order of minutes.

RÉSUMÉ

Le rapport présente l'examen critique des analyses menées par Ontario Hydro sur les températures du combustible et des tubes de force, le comportement du combustible, le rejet de produits de fission et l'intégrité des tubes de force en cas de grosses ruptures entraînant une perte de caloporteur, à la centrale Bruce A ou Pickering A. Lorsqu'on prévoit de faibles débits de vapeur s'échelonnant sur quelques minutes, on ne peut déterminer que de façon incertaine les températures maximales du combustible et le rejet des produits de fission, de même qu'on ne peut garantir l'intégrité des tubes de force.

PREFACE

In 1981, Ontario Hydro submitted new analyses of the consequences of postulated large break loss-of-coolant accidents (LOCA) for Bruce A and Pickering A (Ontario Hydro reports 81038 and 81157) to account for the potential phenomena associated mainly with large break LOCA called pressure tube ballooning, or pressure tube radial straining. These analyses are intended to demonstrate that a ballooned pressure tube will not rupture and include revised predictions of fuel behaviour, fission product releases and doses to the public.

A notable feature of the new analyses is that they do not take account of the cooling capability of the emergency core cooling system (ECCS); instead, the moderator system is relied upon to remove the heat generated in the fuel channel. This approach is different from traditional analyses which were previously used to predict the performance of the ECCS.

In addition to an internal review of these analyses by AECB staff, two contracts were awarded to IDEA Research (DSS Contracts 02SQ.87055-3-4015 and 02SQ.87055-3-4033) to carry out an independent and more detailed review of certain aspects of these analyses; namely, fuel and fuel channel behaviour at high temperatures and fission product release mechanisms.

This report provides a comprehensive summary of several reports submitted to the AECB by the contractor.

A SUMMARY OF THE ASSESSMENT OF FUEL BEHAVIOUR, FISSION PRODUCT RELEASE AND PRESSURE TUBE INTEGRITY FOLLOWING A POSTULATED LARGE LOSS-OF-COOLANT ACCIDENT - EXECUTIVE SUMMARY

The loss of coolant accident (LOCA) analyses for large breaks carried out by Ontario Hydro for Bruce A and Pickering A have been reviewed critically to determine whether the activity source terms represent reasonable upper limits to fission product release and whether pressure tube integrity is assured.

The timing and extent of fission product release in a large break LOCA is governed by the severity and duration of fuel temperature transients and by the characteristics of fission product release mechanisms. In Bruce A and Pickering A it is difficult to support with confidence the determination of maximum fuel temperatures. This is due to the uncertainties associated with the assessment of the following factors:

i) the amount of heat addition or heat removal that occurs during the "blowdown" period;

ii) the time at which, and the extent to which the emergency coolant becomes effective in keeping the fuel cool (what steam flow per channel can be supported confidently?);

iii) the amount of pressure tube deformation that occurs and whether the deformation mode is "ballooning" (ie. good heat removal from the fuel to the moderator) or "sag" (ie. poor heat removal from the fuel to the moderator) or some combination of ballooning and sag (how much pressure tube ballooning, and therefore good heat removal to the moderator, can be credited?);

iv) the behaviour of high temperature steam/hydrogen mixtures in deformed fuel channels (to what extent will pressure tube ballooning cause steam flow in the channel to bypass the interior of the fuel bundles and therefore limit the extent to which the exothermic Zircaloy-steam reaction can occur?);

v) the effect of fuel bundle deformation on heat removal from a channel (to what extent will fuel bundle slumping cause flow to bypass the interior of the fuel bundles and similarly limit the extent of the exothermic Zircaloy-steam reaction?);

vi) the rate at which the exothermic Zircaloy-steam reaction is predicted to occur (what is the oxidation rate of Zircaloy at temperatures near and beyond the Zircaloy melting temperature?); and

vii) the effect of channel material properties on the rate of heat removal from the channel (will Zircaloy emissivities be reduced at extreme temperatures and therefore reduce the rate of radiation heat removal from the fuel and/or will fuel microcracking due to transient gas release reduce the thermal conductivity of the fuel and therefore the rate that heat can be removed from the fuel?).

The characteristics of the various activity release mechanisms that operate at high temperature are not well understood. Does high temperature release of fission products from the fuel grains occur through single atom diffusion or through bubble mobility? If the latter, can the process be modelled reasonably as a single atom diffusion process? What variables affect the timing and extent of microcracking during a transient and how might this affect subsequent releases?

In view of the uncertainties on temperature predictions and release mechanisms, it is very difficult to have confidence that predictions of additional activity release are indeed reasonable upper estimates, for LOCA fuel temperature transients in excess of approximately 1700 C. Therefore, the activity release source terms predicted by Ontario Hydro for large break LOCAs in Bruce A or Pickering A could be considerably underestimated (ie. an order of magnitude).

In the large break LOCA analyses for Bruce A and Pickering A, pressure tube integrity cannot be assured until better analytical assessments coupled with experimental data are provided on the following pressure tube failure mechanisms:

i) hydrogen embrittlement (the potential for rapid hydrogen absorption into pressure tubes at elevated temperatures and the detrimental effect of this on pressure tube ductility and strength at lower temperatures needs to be assessed);

ii) local overstrain caused by localised transverse strain of a pressure tube in a preferentially overheated region (can thermal or mechanical interaction between the fuel and the pressure tube occur and cause local pressure tube overheating prior to uniform ballooning contact between the pressure tube and the calandria tube?); and

iii) pressure tube melting (pressure tube melting can be predicted to occur depending on the assumed channel conditions; how probable are those channel conditions which could lead to pressure tube melting?).

Recommendations have been provided for further experimental work, model development and analytical assessments to improve the understanding of fuel, fission product and pressure tube behaviour in large break LOCAs in Bruce A and Pickering A.

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A. INTRODUCTION

IDEA Research has completed an assessment for the Atomic Energy Control Board of the core behaviour aspects of the Ontario Hydro large break LOCA analyses for Bruce A (1)* and Pickering A (2) nuclear generating stations (NGS). The assessment was performed under contracts 02SQ.87055-3-4015 and 02SQ.87055-3-4033. The major findings of the assessment are summarised in this report.

The assessment objective is discussed in the next section. An in-depth discussion of the objective, scope and content of the assessment is described as phase I work in reference 3. The major findings of the assessment are discussed under the headings of fuel and pressure tube temperatures, fission product release, pressure tube integrity and hydrogen evolution in sections C, D, E and F respectively. Recommendations for further experimental work, model development and analyses to improve the present understanding of core behaviour in large break LOCAs are summarised in section G.

Complete discussions of the work performed for the assessment can be found in references 4 through 7 inclusive.

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* Numbers in ( ) indicate references in section H.

B. ASSESSMENT OBJECTIVE

The objective (3) of the assessment was to identify and to study selectively those factors which, following a large break LOCA in Bruce A or Pickering A, could:

i) lead to a significant (e.g. a factor of three or greater) change in the estimate of the timing and extent of fission product release from the fuel;

ii) imperil the integrity of the pressure tube either before or after pressure tube/calandria tube contact due to pressure tube ballooning, sag or any combination of ballooning and sag; and

iii) lead to a significant change in the estimate of the timing and extent of hydrogen evolution.

The achievement of the overall objective was ensured by the successful completion of the following five tasks.

i) The methods, boundary conditions, assumptions, experimental support and major results of the large break LOCA analyses for Bruce A and Pickering A were reviewed critically (4). Selected supporting documentation (8-16) for Ontario Hydro large break LOCA analyses, which dealt with fuel, fission product and pressure tube behaviour, was included in the review (4).

ii) The status of Canadian and relevant international research and development programmes which study fuel, fission product or pressure tube behaviour during large break LOCAs was summarised (6).

iii) The models and methods used by Ontario Hydro to evaluate fission product distribution in CANDU fuel were reviewed critically (5).

iv) The models and methods used by Ontario Hydro to evaluate fission product release from CANDU fuel were reviewed critically. Various models available outside Canada to predict transient fission product release from UO2 fuel were examined (5).

v) The models and methods used by Ontario Hydro to evaluate fuel and pressure tube behaviour during large break LOCAs were selectively reviewed (7). An independent assessment of fuel and pressure tube behaviour and fission product release was provided which is supported by hand calculations, computer code calculations and results from other core behaviour analyses (17).

C. FUEL AND PRESSURE TUBE TEMPERATURES

The prediction of fuel and pressure tube temperatures in large break LOCAs are important for the following reasons.

i) Fuel temperature affects the timing and extent of fission product release.

ii) Fuel temperature affects the timing and extent of hydrogen evolution from the exothermic reaction between steam and the Zircaloy in a fuel bundle.

iii) Fuel temperature affects the mechanical behaviour of a fuel bundle. Fuel bundle deformation could lead to contact between the bundle and the pressure tube. Bundle/pressure tube contact could result in overheating and possible failure of the pressure tube.

iv) Pressure tube temperature affects the nature (i.e. transverse and/or longitudinal strain) and extent of pressure tube mechanical deformation. Deformation that is dominated by transverse strain (i.e. pressure tube ballooning) may produce complete and relatively uniform contact between the pressure tube and calandria tube. This can result in significant heat transfer from the fuel to the moderator. In contrast, deformation that is dominated by longitudinal strain (i.e. pressure tube sag) results in less heat transfer from the fuel to the moderator than does the ballooning case. This is due to the limited extent of circumferential contact between the pressure tube and the calandria tube. Thus, pressure tube temperatures can affect the extent of contact between the pressure tube and the calandria tube, thereby influencing the rate of heat removal from the fuel and hence fuel temperatures.

v) Pressure tube temperature affects the following pressure tube failure mechanisms.

a) The rates at which hydrogen or oxygen are absorbed into the pressure tube are governed mainly by temperature. Hydrogen or oxygen absorption could result in embrittlement and possible failure of a pressure tube.

b) When the pressure tube temperature exceeds the melting point of zirconium-2.5 wt% niobium, pressure tube failure could occur depending on the oxygen content and consequent strengthening of the pressure tube.

c) Local overheating and/or circumferential temperature gradients could result in local overstrain and failure of a pressure tube.

vi) Pressure tube temperature affects the timing and extent of hydrogen evolution from the exothermic reaction between steam and the Zircaloy in the pressure tube.

It is difficult to make confident predictions of the severity and duration of fuel and pressure tube temperature transients in large break LOCAs in Bruce A and Pickering A because of the uncertainties associated with the determination of:

i) the timing and extent of heat addition and removal during the blowdown period;

ii) the effectiveness (timing and extent) of emergency coolant injection (ECI);

iii) the nature and extent of pressure tube deformation;

iv) the behaviour of steam/hydrogen mixtures in a deformed CANDU fuel channel (i.e. flow bypass, hydrogen absorption versus heat removal);

v) the effect of fuel bundle deformation on heat removal from a CANDU fuel channel;

vi) the rate of the exothermic Zircaloy-steam reaction; and

vii) the effect of temperature dependent fuel and pressure tube material properties on heat removal from a CANDU fuel channel.

The uncertainties associated with these previous seven factors are discussed in Subsections C.1 to C.7 inclusive.

1. Heat Addition and Removal During Blowdown

Normally Ontario Hydro would use the computer code SOPHT to predict the timing and extent of heat removal during a large break LOCA.

Ontario Hydro did not use SOPHT directly in their analyses of large break LOCAs for Bruce A and Pickering A. In their analyses, the accident was divided in time into an initial blowdown heat removal period and a subsequent steam cooling period. For Bruce A and Pickering A the blowdown period was assumed to last 5 and 10 seconds respectively even though system depressurisation was more rapid in Pickering A.

For the region of the core where flow was expected to be stagnated, fuel temperatures at the beginning of the steam cooling period were determined empirically from:

i) the average fuel temperatures at the beginning of the blowdown period as calculated by the computer code HOTSPOT-II;

ii) modified by heat addition to the fuel due to the neutronic power pulse;

iii) modified by heat addition to the fuel as a result of decay power; and finally

iv) modified by heat removal from the fuel as a result of blowdown cooling.

The parameters which affect this empirical method of calculating fuel temperatures at the beginning of the steam cooling period were less restrictive for Pickering A than for Bruce A. If assumptions consistent with those made for Bruce A had been made in Pickering A, then the fuel temperatures at the beginning of the steam cooling period in Pickering A would have been higher than those given in reference 2.

Many factors can affect system thermohydraulic conditions, and consequently fuel temperatures, during a large break LOCA. A critical review of the technical validity of, and experimental support for, the use of computer codes such as SOPHT, FIREBIRD and RAMA to model this situation was beyond the scope of the present assessment (3). However, even if the empirical method used by Ontario Hydro to calculate fuel temperatures at the beginning of the steam cooling period is accepted in principle, the following concerns with the details of the approach still exist:

i) average fuel temperatures under normal operating conditions as predicted by HOTSPOT-II can be as much as 150C lower than those calculated by the more widely accepted fuel behaviour code ELESIM-II(MOD9);

ii) for Bruce A, the energy deposition averaged over all the fuel in the core (3.1 full power seconds, FPS) due to the neutronic power pulse was used in the calculation of fuel temperatures at the beginning of the steam cooling period, rather than the energy deposition in the "hot bundle" (3.8 FPS); and

iii) for Pickering A the neutronic power transient was calculated with the single most effective shutoff rod (SOR) not available; a more generally accepted assumption is that the two most effective SORs are unavailable.

Until these concerns have been addressed, it must be concluded that the fuel temperatures at the beginning of the steam cooling period as calculated by Ontario Hydro for Bruce A and Pickering A are underestimated. Thus, there will be more stored energy in the fuel at the beginning of the steam cooling period than is predicted. This will affect the determination of the severity, extent and duration of fuel overheating during the steam cooling period.

2. Timing and Extent of ECI Effectiveness

As indicated previously, Ontario Hydro did not use a system thermohydraulics computer code to determine the timing and extent of ECI effectiveness in the Bruce A and Pickering A analyses. Instead, the channels were characterised as "early", "delayed" or "late" heatup channels. Early heatup channels were those channels where little heat removal occurred during the blowdown period and therefore fuel temperatures at the beginning of the steam cooling period were relatively high. Late heatup channels were assumed to experience effective heat removal during the blowdown period and therefore fuel temperatures at the beginning of the steam cooling period were quite low. Delayed heatup channels were assumed to fall in between early and late heatup channels. At the end of the blowdown period the channel conditions were assumed to be as follows:

	Early Heatup Channels		Late or Delayed Heatup Channels	
	Bruce A	Pickering A	Bruce A	Pickering A
Number of Channels	240	98	240	98
Blowdown Period	0-5s	0-10s	0-100s	0-25s
Initial Fuel Temperatures (C)	300-1600	400-1700	250	200-1100
Inlet Steam Conditions: -Flow(g/s)	100	100	100	1000(0-25s) 200(>60s) exp.decay(25-60s)
-Temperature (C)	300	Saturation	200	Saturation

These channel conditions were provided as input to the CHAN-II(MOD3) computer code (9,18) which was used to predict fuel and pressure tube temperatures during the steam cooling period. The peak fuel temperature in the maximum power early heatup channels for both Bruce A and Pickering A was approximately 2400 C (1,2).

Ontario Hydro observed that the peak fuel temperature in a maximum power (7.5 MW) early heatup channel in Bruce A increased by only 100 C when the inlet steam flow was reduced from 100 g/s to 25 g/s (1). This observed insensitivity of peak fuel temperature to inlet steam flow can be attributed to the fact that the exothermic Zircaloy-steam reaction and convective heat transfer were assumed not to occur over almost all of the overheated section of the channel (7). The changes in peak fuel temperatures, therefore, were the result of differences between the rates of decay power heat generation and radiation heat removal, neither of which are affected by inlet steam flow. Peak fuel temperatures as predicted by CHAN-II(MOD3) were observed to be extremely sensitive to inlet steam flow when the exothermic Zircaloy-steam reaction and convective heat transfer were allowed to occur throughout the channel (7). For example, the peak fuel temperatures in a 7.5 MW, early heatup channel of Bruce A were approximately 3000 C and 2200 C for inlet steam flows of 15 g/s and 100 g/s respectively (7).

CHAN-II is a fairly simple, assumption driven, quasi-steady state computer code which models the fuel as concentric rings (4). Due to the simple nature of its fuel model, CHAN-II is best applied to situations where the temperature profile across the diameter of any fuel element is fairly flat (18). Fuel temperature diametral profiles will not be flat during the first 10 seconds of a LOCA. Therefore, in both the Bruce A and Pickering A analyses the CHAN-II computer code was used at too early a time in the LOCA to predict fuel and pressure tube temperatures properly (4).

In 1983 experiments began at Whiteshell Nuclear Research Establishment (WNRE) in an attempt to verify selected submodels of the CHAN-II computer code (6). To date the experimental information has been produced by a relatively simple arrangement using a Zircaloy sheathed electric heater inside a Zircaloy tube. At present there is little relevant experimental data available against which the ability of the CHAN-II computer code to predict fuel and pressure tube temperatures can be verified, for either a normal or a deformed channel geometry.

The prediction of fuel and pressure tube temperatures under steam cooling conditions in a LOCA will be uncertain if the inlet flow conditions to all channels cannot be estimated with confidence. Similar uncertainty will be present if the predictive capability of the CHAN-II computer code remains experimentally unverified.

3. Nature and Extent of Pressure Tube Deformation

The severity and duration of fuel temperature transients will be affected by the rate and extent of heat removal through the pressure tube and calandria tube to the moderator. Pressure tube sag due to longitudinal strain, or pressure tube "slumping", due to localised deformation around the garter springs results, at most, in limited contact between the pressure tube and the calandria tube (6). This provides a relatively poor heat removal path to the moderator. Pressure tube ballooning, due to transverse strain, can result in complete circumferential contact between the pressure tube and the calandria tube. This can provide a good heat removal path to the moderator if the exterior surface of the calandria tube does not experience extensive dryout. Therefore, in order not to underestimate the severity and duration of fuel temperature transients, the rate at which pressure tube ballooning develops and the extent to which this ballooning occurs along the channel must not be overpredicted.

The parameters which influence the rate and extent of pressure tube ballooning are the channel depressurisation transient, the pressure tube temperature transient, the pressure tube circumferential temperature gradient and the rate at which the pressure tube material strains as a function of temperature, stress and microstructure. Ontario Hydro's treatment of these parameters could result in an underestimation of fuel temperatures. For example, in the analyses of large break LOCAs in Bruce A (1) and Pickering A (2), Ontario Hydro used depressurisation transients for the 25% Reactor Inlet Header (RIH) and 45% RIH breaks, respectively. Larger breaks would result in faster depressurisation transients and less pressure tube ballooning if all other controlling parameters remained the same.

Also, Ontario Hydro assumed that pressure tube overheating began at the very start of the LOCA and that the pressure tube temperature transients were of the form $(1 - \exp(-t))$. As the initiation of pressure tube overheating is delayed in time, the potential for pressure tube ballooning decreases if all other controlling parameters remain the same.

There is no directly relevant experimental data available to verify when and how fast pressure tube overheating will occur in a large break LOCA.

Finally, Ontario Hydro increased the transverse strain rate, as calculated by the strain rate equations available at the time the analyses were performed, by a factor of 7 over the pressure tube temperature range 575 to 925 C (1,2). As a result, if pressure tube temperatures exceeded approximately 600 C for channel pressures in excess of 2 MPa, then the rate of transverse strain was quite rapid. The rationale for the factor of 7 (1,2) was to account for the influence of pressure tube microstructure (i.e. grain size) on the transverse strain rate, as calculated from equations derived from uniaxial isothermal test data (6). Experimentally verified transverse strain rate equations are now available which account for the effect of microstructure directly (6). The effect, on pressure tube deformation behaviour, of using these more recent equations instead of the factor of 7, should be evaluated.

The end result of Ontario Hydro's treatment of pressure tube deformation is that ballooning is the only mode of deformation assumed to occur in early heatup channels (1,2). Also, the times at which pressure tube/calandria tube contact occurs due to pressure tube ballooning are quite early and the axial extent of contact quite large, as summarised in Table 1. Note that the timing of pressure tube/calandria tube contact is earlier and the extent of contact is greater for Pickering A than Bruce A, even though:

i) the depressurisation transient for Pickering A is more rapid than for that Bruce A; and

ii) the Zircaloy-2 pressure tubes in Pickering A Units 1 and 2 would be expected to strain more slowly than the Zr-2.5 wt% Nb pressure tubes in Bruce A for the same temperature and channel pressure. This is a consequence of the temperature for the alpha to alpha plus beta phase transformation being approximately 20OC higher for Zircaloy-2 than for Zr-2.5 wt% Nb.

The strain rate is also lower because the Zircaloy-2 pressure tubes are approximately twenty percent thicker than the Zr-2.5 wt% Nb pressure tubes. Therefore, the same channel pressure leads to a lower wall stress in the Zircaloy-2 pressure tubes.

The more severe power pulse associated with Pickering A results in fuel heatup which is faster and axially more extensive than in Bruce A. As a result, for nomially similar heat transfer conditions in a channel, pressure tube heatup will be faster and axially more extensive for Pickering A than for Bruce A. Therefore, faster and more heat transfer from the fuel to the moderator is predicted for Pickering A than for Bruce A.

If an early heatup channel experienced pressure tube slumping or sag rather than ballooning, heat transfer to the moderator would be reduced and the maximum fuel temperatures could increase by several hundred degrees C for low steam flows (7). In the Ontario Hydro analyses, pressure tube slumping was not considered and pressure tube/calandria tube contact over a 120 degree angle was assumed to occur due to sag if the pressure tube temperature reached 1000 C. Only delayed or late heatup channels were assumed to experience pressure tube sag. Large scale sag experiments have shown that pressure tube/calandria tube contact due to slumping will occur if the pressure tube temperature reaches 850 C (6). The experiments also showed that the effective contact angle between the pressure tube and calandria tube due to slumping or sag is approximately 30 degrees (6). Therefore, a combination of slumping and sag, (rather than pressure tube sag alone) with limited heat transfer to the moderator, will be the alternative deformation mode to pressure tube ballooning.

A reassessment of pressure tube deformation behaviour during a large break LOCA in Bruce A and Pickering A is recommended:

i) to determine whether pressure tube slumping/sag, rather than ballooning, could occur in early heatup channels; and

ii) to account for pressure tube slumping as a deformation mechanism and determine its effect on maximum fuel temperatures, especially for early heatup channels.

Also, the sensitivity of fuel temperature transients to the assumptions made about the nature and extent of pressure tube deformation in the early heatup channels of Pickering A should be investigated.

4. Steam/Hydrogen Behaviour in a Deformed Fuel Channel

Ontario Hydro has assumed in their analyses (1,2) that if pressure tube ballooning occurs over a segment of a channel, then the exothermic Zircaloy-steam reaction and convective heat transfer would not occur in the interior of the fuel bundles in that segment. The assumption is based on the expectation that a low resistance flow path will be provided by the space created above the fuel bundles as the pressure tube expands. Consequently, it is argued that no steam will flow through the interior of the fuel bundles (14). In the early heatup channels, pressure tube ballooning was predicted to occur over almost all of the region where sheath temperatures were high enough for the exothermic Zircaloy-steam reaction to occur (1,2). As a result, a negligible amount of heat from the exothermic Zircaloy-steam reaction was generated in the early heatup channels (i.e. approximately 3 MJ for a 7.5 MW channel in Bruce A) (7).

In contrast, if the exothermic Zircaloy-steam reaction and convective heat transfer are allowed to occur throughout the fuel bundles in a ballooned channel at low steam flows (i.e. 0-20 g/s), the amount of heat generated due to the Zircaloy-steam reaction is much greater (i.e. approximately 90 MJ for a 7.5 MW channel in Bruce A). In this case, the maximum fuel temperatures increase by several hundred celcius degrees (7) as compared to the Ontario Hydro analyses.

There is no experimental data available to verify the assumption that steam will not access the interior of a fuel bundle in the ballooned region of a channel (6). The prediction of maximum fuel temperatures is extremely sensitive to this assumption (7). As a result, the assumption should not be made until well supported by relevant experimental data on the behaviour of high temperature steam/hydrogen mixtures in deformed fuel channels where fuel temperatures are in the range 1500-3000 C.

In the Ontario Hydro analyses (1,2) the hydrogen gas generated due to the Zircaloy-steam reaction is assumed to be available to remove heat from the channel (9, 18). At low inlet steam flows, all the steam can be consumed by the upstream fuel bundles due to the Zircaloy-steam reaction (7). As a result, only hydrogen is available to remove heat from the downstream fuel bundles. Hydrogen absorption by the Zircaloy channel components would result in less heat removal from the downstream fuel bundles and therefore higher downstream fuel temperatures (7). Relevant experimental data is required on the potential for hydrogen absorption in Zircaloy at elevated temperatures.

5. Effect of Fuel Bundle Deformation on Heat Removal

Ontario Hydro has assumed in their analyses (1,2) that if the temperature reaches 1850 C anywhere in a fuel bundle then the bundle would be in a slumped configuration with a 120 degree contact angle and a 2 kW/m2C heat transfer coefficient between the bundle and the pressure tube. Further, it was assumed that neither the exothermic Zircaloy-steam reaction nor convective heat transfer would occur in the interior of a slumped fuel bundle or in the 120 degree contact zone. The rationale for this assumption was that negligible steam access to the bundle would occur as a result of increased flow resistance due to bundle deformation.

The timing and extent of fuel bundle slumping is summarised in Table 2 for the early heatup channels of Bruce A and Pickering A (1,2). Bundle slumping was predicted to occur much earlier and was more extensive in Pickering A than in Bruce A even though more blowdown heat removal was credited in Pickering A. Experimental data on horizontal, in-reactor, high temperature fuel behaviour is non-existent (6). The most relevant out-reactor, horizontal data to date indicates that oxidation strengthening of Zircaloy coupled with the high melting temperature of zirconium dioxide could cause fuel bundle geometry to remain relatively normal at temperatures in excess of 2000 C (6). Also, there is no relevant experimental data available to verify that steam will not access the interior of a deformed fuel bundle at low flows.

In the calculation of large break LOCA fuel temperatures it should be assumed that steam access to the interior of a fuel bundle will not be impeded at any temperature until relevant experimental data is available to support behaviour to the contrary. Similarly, heat removal via solid contact between the fuel bundle and the pressure tube should not be credited.

6. The Exothermic Zircaloy-Steam Reaction

The exothermic reaction between Zircaloy and steam may be represented by the overall equation:

$$Zr + 2H_2O \longrightarrow ZrO_2 + 2H_2 + 6.4 \text{ MJ per kg of Zr consumed.}$$

In the large break LOCA analyses for Bruce A (1) and Pickering A (2), Ontario Hydro used the equations developed by Urbanic and Heidrick (6) to determine the rate at which the Zircaloy-steam reaction would occur on the fuel sheaths and the pressure tubes. The following assumptions made by Ontario Hydro also influence the rate at which heat is added to the core due to the Zircaloy-steam reaction:

i) the Zircaloy-steam reaction occurs only on the exterior surface of the fuel sheaths;

ii) the Zircaloy-steam reaction is governed by parabolic oxidation kinetics;

iii) the oxidation rate for sheath temperatures in excess of the Zircaloy melting temperatures is equated to the rate at the Zircaloy melting temperature; and

iv) the thickness of Zircaloy consumed is equal to the thickness of zirconium dioxide formed.

Also, in all versions of the CHAN-II computer code (9,18) there was an error in the determination of the centre element fuel temperature. The amount of heat generated due to the Zircaloy-steam reaction on the centre element was subtracted rather than added when the centre element fuel temperature was determined.

Fuel temperatures in a large break LOCA will be affected by the amount of heat generated due to the Zircaloy-steam reaction and the rate at which it is generated. When the previous factors are combined with the assumptions made about turning off the Zircaloy-steam reaction in the interior of a fuel bundle, the result is that very little heat is generated from the Zircaloy-steam reaction in the Bruce A and Pickering A analyses. For example, a total of only 3.4 MJ of heat due to the Zircaloy-steam reaction is released in the first 500 seconds in a 7.5 MW channel in Bruce A, where the temperature exceeds 1000 C over a large portion of the channel. In a Bruce A fuel channel, there is the potential to generate 190 MJ of heat if all the Zircaloy in the fuel bundles oxidise and 390 MJ of heat if the pressure tube oxidises completely. The factors which will affect the determination of the rate and extent of the Zircaloy-steam reaction will now be discussed.

Parabolic reaction rate constants for Zircaloy oxidation as determined by Urbanic-Heidrick, Baker-Just, Cathcart and Leistikow et al, are given in Figure 1 (7). It can be seen that the oxidation rates determined by Urbanic-Heidrick are low for temperatures greater than 1400 C compared to the results of the other workers. The results of the most recent work of Leistikow et al (19) indicate that at temperatures of 1600 C, Zircaloy oxidation rates are best represented by the Baker-Just correlation.

In the work of Urbanic-Heidrick, it was assumed that Zircaloy-4 would melt at the melting point of zirconium, i.e. 1850 C. Recently, the melting point of Zircaloy-4 has been determined experimentally to be 1760 C. As a result, the Urbanic-Heidrick oxidation rates near the melting point of Zircaloy-4 must be considered suspect. Experiments are to be performed at WNRE to determine oxidation rates near the melting point of Zircaloy-4. There is no experimental data available on oxidation rates beyond the melting point of Zircaloy-4.

The time required for the Zircaloy-steam reaction to convert a Zircaloy-4, CANDU fuel sheath (420 microns thick) completely to zirconium dioxide is given in Table 3 as a function of various assumptions.

If oxidation occurs on both the inner and outer surfaces of the fuel sheath (i.e. double-sided oxidation), then the through-wall oxidation time is reduced by a factor of four compared to single-sided oxidation. In a LOCA, fuel sheath diametral strain and eventual burst failure could allow steam access to the inside of fuel elements and consequent oxidation of the inner surface of the fuel sheaths. Steam ingress into failed fuel elements and inner surface oxidation has been observed in experiments on PWR fuel (7). There is no experimental data on the extent of inner surface oxidation as a function of burst size, magnitude and extent of uniform sheath strain, steam flow rate, steam temperature and sheath temperature for CANDU fuel.

If the oxidation kinetics are linear instead of parabolic, then the through-wall oxidation time is the square root of the oxidation time for parabolic kinetics. Parabolic oxidation kinetics are governed by steam having to diffuse through an intact zirconium dioxide layer in order to react with the Zircaloy surface underneath. As the zirconium dioxide layer gets thicker it takes a longer time for the steam to diffuse through to the Zircaloy surface and the oxidation rate decreases. Linear oxidation kinetics would imply that steam has relatively free access to the Zircaloy surface. Greater access would be provided by cracking or spalling of the oxide layer. There is no experimental data on the mechanical behaviour of zirconium dioxide at elevated temperatures where temperature cycles could result in thermal shock and consequent cracking or spalling of the oxide.

Given that Zircaloy oxidation is allowed to occur, the rate at which it occurs may be underpredicted at temperatures greater than 1400 C and overpredicted for temperatures less than 1400 C, by the method used in the Bruce A and Pickering A large break LOCA analyses. Further experimental work is required to determine oxidation rates at and beyond the melting point of Zircaloy, the mechanical properties of zirconium dioxide at elevated temperatures and the extent to which steam ingress into burst fuel elements can result in oxidation of the inner surface of the fuel sheaths.

7. Effect of Channel Material Properties on Heat Removal

Fuel temperatures in a large break LOCA are governed by the rates at which the various heat addition and heat removal mechanisms occur. The rate at which heat can be removed from the fuel and transferred to the coolant or the moderator is affected by the following channel material properties.

i) The thermal conductivity of the fuel, which determines how rapidly heat can flow to the outer surface of the fuel.

ii) Tne fuel-to-sheath heat transfer coefficient, which determines how rapidly heat can be transferred from the outer surface of the fuel to the inner sheath surface.

iii) The thermal conductivity of the fuel sheath, which determines how rapidly heat can flow through the sheath. The thermal conductivity of zirconium dioxide is an order of magnitude lower than that of Zircaloy.

iv) The emissivities of the exterior surface of the sheath and the inner surface of the pressure tube. The emissivities are especially important if radiation is the main mode of heat transfer from the fuel to the pressure tube.

Fuel thermal conductivity can be reduced by up to 50% due to extensive microcracking of the fuel associated with transient gas release at elevated temperatures (7). In CHAN-II(MOD3) calculations for a 7.5 MW channel in Bruce A, maximum fuel temperatures increased by almost 200 C when the fuel thermal conductivity was reduced to 50% of the values used in the Ontario Hydro large break LOCA analyses (7).

A fuel-to-sheath heat transfer coefficient of 7.0 kW/m2C was used in the CHAN-II(MOD3) analyses performed by Ontario Hydro for Pickering A and Bruce A. Such a value is representative of good contact between the fuel and the sheath which will not be the case once the sheath has strained away from the fuel. The CHAN-II(MOD3) code predictions became unstable (i.e. the centre element sheath temperature alternates between a very large positive and a very large negative number) when the fuel to sheath heat transfer coefficient was reduced from 7.0 kW/m2C. Therefore, the solution logic for the determination of the centre element sheath temperature in the CHAN-II(MOD3) computer code must be considered suspect.

The emissivities of the sheath exterior surface and the pressure tube inner surface were assumed to be 0.8 in the Ontario Hydro CHAN-II(MOD3) analyses. This is the maximum value of emissivity for Zircaloy and represents the value for black oxide. There is little or no data on the emissivity of Zircaloy and zirconium dioxide at temperatures greater than approximately 1300 C. However, fuel workers in the U.S. have developed a correlation for Zircaloy/zirconium dioxide emissivity which predicts a value of 0.325 for temperatures greater than 1500 C independent of oxide layer thickness (20). In CHAN-II(MOD3) calculations for a 7.5 MW channel in Bruce A, maximum fuel temperatures increased by 130 C when the sheath and pressure tube emissivities were reduced from 0.8 to 0.4.

Experimental work should be performed to determine the emissivity of Zircaloy and zirconium dioxide at temperatures greater than 1300 C.

8. Section Closure

A limited sensitivity analysis was performed (7) using the CHAN-II(MOD3) computer code to determine the effect of various assumptions on maximum fuel temperatures in a 7.5 MW channel in Bruce A. The major results are summarised in Table 4.

Because of the assumptions made by Ontario Hydro, the reference case (case 1) has the exothermic Zircaloy-steam reaction and convective heat transfer "turned-off" throughout most of the channel. As a result, the maximum fuel temperature is not sensitive to inlet steam flow. The Ontario Hydro reference case has an inlet steam flow of 100 g/s with a resultant maximum fuel temperature of 2344 C. A reduction in inlet steam flow to 5 g/s results in only a 60 C increase in maximum fuel temperature.

The reference case used for the sensitivity analysis (case 2) is the same as the Ontario Hydro reference case with the exceptions that:

i) the assumption of complete flow bypass has been removed;

ii) the calculation of centre element fuel temperature has been corrected; and

iii) the inlet steam flow is 15 g/s.

With this new reference case, the maximum fuel temperature is now very sensitive to inlet steam flow. For 15 g/s inlet steam flow, the maximum fuel temperature is 2983 C whereas for 100 g/s it reduces to 2221 C.

With the exothermic Zircaloy-steam reaction allowed to occur throughout the channel, the maximum fuel temperature becomes sensitive to a reduction in Zircaloy emissivities, to a reduction in fuel thermal conductivity, to the assumption of double-sided versus single-sided oxidation attack and to the assumption that pressure tube sag occurs rather than ballooning. However, even with all these factors set to maximise fuel temperatures, an increase in inlet steam flow to 100 g/s results in a reduction of over 800 C in predicted peak fuel temperatures.

Based on the sensitivity studies carried out using the modified version of CHAN-II(MOD 3), maximum fuel temperatures are sensitive to the following factors in order of decreasing importance:

i) inlet steam flow;

ii) the potential for flow bypass due to pressure tube ballooning or bundle slumping;

iii) the deformation mode of the pressure tube (i.e. sag versus ballooning); and

iv) fuel thermal conductivity, double-sided versus single-sided oxidation and Zircaloy emissivity.

Until the effects of these and other factors can be well characterised, the confident prediction of a reasonable upper limit to maximum fuel temperatures under prolonged low steam flow conditions in large break LOCAs is impossible. Therefore, the large break LOCA fuel temperature predictions provided by Ontario Hydro for Bruce A (1) and Pickering A (2) should not be considered either accurate or an "upper bound".

D. FISSION PRODUCT RELEASE

The prediction of the timing and extent of fission product release from the fuel in a large break LOCA is important because it can affect the calculated dose to the public. The timing and extent of fission product release from the fuel is affected by the following factors:

i) the timing and extent of fuel sheath failures;

ii) the fuel heatup rate;

iii) the magnitude and duration of the peak fuel temperature; and

iv) the distribution of fission products (i.e. free, grain boundary and grain-bound inventories) in the fuel under normal operating conditions.

Along with the uncertainties in the prediction of these factors, there are also uncertainties associated with the modelling of activity release mechanisms. This situation makes it difficult to determine, with confidence, a reasonable upper limit for fission product release from the fuel under prolonged low steam flow conditions in a large break LOCA.

The uncertainties associated with the determination of fuel temperature transients were discussed in section C. The uncertainties associated with the determination of fission product distribution in the fuel and the modelling of activity release mechanisms are discussed in sections D.1 and D.2 respectively.

Large break LOCA source term estimates for Bruce A, for a range of assumptions on fuel temperatures and activity release mechanisms, are discussed in section D.3.

1. Fission Product Distribution in Fuel

In fuel under normal operation, the heat produced due to fission results in a characteristic and predictable temperature distribution across the fuel element. At the same time, there is some distribution of fission products in the fuel at a gross level (on the scale of the pellet) and also at a detailed level on the scale of the fuel grains.

Fission products generated in the fuel grains diffuse to the grain boundaries under the concentration gradient that becomes established across the individual grains. As a result, fission products build up on the grain boundaries, and some of this built up inventory may leave the UO2 altogether through tunnels and cracks that form in the fuel. Although lost from the UO2, this portion of the fission product total inventory remains in the free spaces around the UO2 within the fuel sheath. Prediction of the resulting distribution of fission products (on the small and large scales) is not a simple problem because of the number of factors that affect fission product movement within the fuel. Some of these factors are fuel temperature, which varies with burnup as well as spatially across the fuel element, initial location of the fission products in the element, fuel power history and fission product species.

The most important of the above factors is fuel temperature and this, in turn, is affected by a large number of other factors. However, it is generally felt that fuel temperature predictions under normal operating conditions can be made quite reliably and that the overall situation is reasonably well understood. As a result, a number of computer codes exist for predicting fuel temperature and its effect on stable fission product gas release under normal operating conditions. For CANDU fuel, the standard code is ELESIM-II (MOD 9).

In their predictions of fission product distribution in fuel, Ontario Hydro has used ELESIM as the starting point. By making assumptions that relate the behaviour of unstable fission products to that of stable fission gas, a set of equations describing fission product loss from the grains and loss outside the grains can be simplified and solved. The solution of these equations yields the amounts of fission products that are retained within the fuel grains. That fraction that leaves the grains is assumed to be distributed between the grain boundary and the free inventories.

The major assumptions used in the calculations described in the above paragraph are:

i) the average concentration of a given unstable species can be represented as a fraction of the average stable fission gas concentration over the grain;

ii) loss of fission products to the grain boundaries is by single atom diffusion;

iii) all isotopes diffuse at the same rate;

iv) at any point in the fuel, local burnup can be represented by element average burnup; and

v) the fuel operates at constant power.

Assumption i) is essential to the model since without it the equations cannot be solved. However, it is without clear support.

Assumption iv) may result in substantial errors since the burnup in the fuel at a specific point is not the same as the average element burnup. As burnup proceeds, this difference increases, with fuel in the lower temperature regions of the pellet reaching higher than average burnup, and higher temperature fuel reaching lower than average burnup. The size, and to some extent, the nature of the resulting errors that would appear in the Ontario Hydro model are difficult to estimate.

Since fuel does not operate at constant power over its burnup range, contrary to assumption v), a further error will result. The nature and size of this error are impossible to estimate.

The portion of the total fission product inventory that escapes from the fuel grains is divided between the free inventory and the grain boundary inventory in the Ontario Hydro model. Using fission product retention data from Chalk River Nuclear Laboratories (CRNL) (5), and the predicted total release from the grains given by the Ontario Hydro model, a fraction is derived, which, when applied to the predicted release from the grains, gives the amounts of fission products residing on the grain boundaries. The remainder constitutes the free inventory.

Comparison of this predicted free inventory with experimental measurements from CRNL indicates apparently reasonable agreement. However, this says nothing about the grain boundary inventory, which remains unverified. Furthermore, a less optimistic interpretation of the CRNL fission product retention data would change both the predicted free and grain boundary inventories. The validation of the free inventory prediction therefore can be questioned.

At least the following should be provided to answer the concerns arising from this review:

i) a full study, with discussion, of the sensitivities of the fission product distribution model;

ii) a demonstration of the effect on model predictions that the use of local burnup would have;

iii) full discussion of the uncertainties in, and the use made of, the CRNL fission product retention data; and

iv) documentation of the coded version of the Ontario Hydro fission product distribution model.

2. Activity Release Mechanisms

During an accident, fission products that are released from the fuel may come from the free inventory, the grain boundaries or the bound inventory. Some of the mechanisms affecting these releases are considered in the following.

Release of the free inventory depends on failure of the fuel sheath; sheath failure mechanisms will not be discussed here since they are beyond the scope of the present work. However, release of free inventory is usually assumed to be complete on sheath failure. Sheath failure is also necessary for release from the fuel of the other fission product inventory components.

In the Bruce A and Pickering A analyses, the only transient release mechanisms that were applied are:

i) diffusional release from the fuel grains;

ii) release at high temperature due to grain boundary separation; and

iii) release of grain boundary inventory due to fuel powdering on rewet.

The diffusional release model used in the CURIES (MOD 1) code, which was used for the Bruce A and Pickering A analyses, is the same as that present in an earlier version of the code, CURIES. This is a relatively simple model dependent only on time and temperature and was derived from data obtained from operational transients at CRNL. Note that the CURIES (MOD 1) code is not documented and there is no longer an active version of the code in existence.

A more recent version of CURIES (MOD 1), called CURIES-II, contains a different diffusional release routine that is claimed to be based on data from experiments performed at Argonne National Laboratory. These experiments were carried out on irradiated fuel. As shown in Figure 2 CURIES-II predicts much higher diffusional releases than CURIES (MOD 1) for temperatures greater than 1900 C and lower diffusional releases for temperatures less than 1900 C.

Releases of grain boundary inventory at high temperature due to grain separation are assumed to be complete at temperatures equal to or greater than 2400 K. At temperatures below this it is assumed no release from the grain boundary inventory takes place.

On rewet, 10% of the grain boundary inventory is released from fuel at temperatures below 1373 K, rising linearly to 100% at temperatures greater than or equal to 1973 K.

The Ontario Hydro analyses predict that the vast majority of the total fission product inventory is present in the grains, considering the core as a whole. Therefore, a small change in the predicted fractional release from this component could mean a large change in the absolute value of the release. The very different nature of the predicted releases given by the models in CURIES (MOD 1) and CURIES-II, and the magnitude of the fuel temperature uncertainties described elsewhere in this report indicate that large changes in release predictions are indeed possible. Also, the curve used by Ontario Hydro to obtain the diffusion coefficient as a function of temperature actually refers to a bubble diffusivity and has therefore been misappropriated. Finally, the release predictions from neither CURIES (MOD 1) nor CURIES-II have been validated against experimental data.

The all-or-nothing criterion for release of grain boundary inventory at 2400 K is difficult to rationalise and is without firm support. Work done using the FASTGRASS code indicates that considerable grain separation and hence fission product release can occur at temperatures below 2400 K.

3. Source Term Estimates

In the large break LOCA analysis for Bruce A, Ontario Hydro predicted that a total of 1.6 MCi of I-131 would be released from the fuel. Almost all of the release came from the early heatup channels. Ontario Hydro also predicted (1) that the total core inventory of I-131 (78 MCi) would be distributed in the fuel as follows:

Free inventory = 2.7 MCi

Grain boundary inventory = 1.4 MCi

Grain-bound inventory = 73.9 MCi

Therefore, the total release of I-131 from the fuel was predicted to be just slightly more than the free inventory of half the core.

Release predictions from FASTGRASS during fuel heatup (refer to Figure 3) and the experimental information of Hofmann on the dissolution of UO2 due to the interaction between molten Zircaloy and UO2 have been used to provide independent estimates of the half-core activity release for a large break LOCA in Bruce A (7). When the fuel temperatures for the early heatup channels in Bruce A are used, the half core release of I-131 is predicted to be in the range of 2.1 - 2.5 MCi as shown in Table 5. When the somewhat more elevated temperatures from the 600 MW LOCA with the coincident loss of emergency coolant injection (LOCA/LOECI) analysis (17) are applied to Bruce A, the half core release of I-131 is predicted to be in the range 4.2 - 6.1 MCi as shown in Table 6. On average the maximum fuel temperatures in the 600 MW LOCA/LOECI analysis were 200 to 300 C higher than those for the Bruce A LOCA analysis. The fuel temperatures from the 600 MW LOCA/LOECI analysis were used to provide an estimate of the effect on activity release estimates for Bruce A of an increase in maximum fuel temperatures over the core.

The activity release estimates given in Tables 5 and 6 are based on the following assumptions.

i) The entire half core free inventory is released. The free inventory is as calculated in reference 1.

ii) The release component due to the Zircaloy/UO2 interaction considers only fuel temperatures in excess of 1750 C which is approximately the melting point of Zircaloy. UO2 dissolution and consequent activity release is assumed not to occur below 1750 C.

iii) There is no release from the fuel due to high temperature diffusion after fuel heatup is complete. In reality, depending on the magnitude and duration of the maximum fuel temperatures, the diffusional release component could be substantial.

iv) The release from the fuel due to fuel powdering on coolant desuperheating and sheath rewet is zero. Ontario Hydro assesses this release component in their analyses of Bruce A and Pickering A. The "rewet release" component, which is assumed to originate only from the grain boundaries, will probably be small compared to the transient and diffusional release components.

Thus, all activity release mechanisms are not accounted for in the source term estimates summarised in Tables 5 and 6. However, these estimates are still greater than the total core release from the fuel predicted by Ontario Hydro for a large break LOCA in Bruce A. This illustrates that the use of different activity release models and/or higher fuel temperatures can result in a considerable increase in predicted activity release. If all activity release mechanisms were accounted for, and fuel temperature predictions of the sort discussed in section C.8 were used in the determination of activity release, the resultant source term would be greater than the estimates given in Tables 5 and 6.

4. Section Closure

The activity release source terms provided by Ontario Hydro in the Bruce A and Pickering A large break LOCA analyses can not be thought of as reasonable "upper limits" for the accident conditions modelled.

Further work is required to characterise in a better manner all the various activity release mechanisms as they relate to CANDU fuel. More importantly, uncertainties affecting the determination of fuel temperature transients need to be dramatically reduced. Only when this is done can reasonable "upper limits" to activity release be predicted more confidently for Bruce A and Pickering A.

E. PRESSURE TUBE INTEGRITY

It is important to ensure pressure tube integrity in large break LOCAs because the assessment of core behaviour with one or more failed pressure tubes becomes highly speculative. With the onset of pressure tube failures, the core geometry starts to degrade and it becomes difficult, if not impossible, to assess the final core configuration with present analytical tools and experimental data. Similarly, fission product releases under these conditions are difficult or impossible to estimate. Thus, large break LOCA analyses must demonstrate that all pressure tubes in the core remain intact.

Any one of the following scenarios could result in pressure tube failure during a large break LOCA.

i) Before complete pressure tube/calandria tube contact occurs, a relatively severe temperature gradient around the circumference of a pressure tube could result in localised overstrain and failure of a pressure tube.

ii) Before pressure tube/calandria tube contact occurs, fuel bundle overheating could result in localised thermal/mechanical interaction between a fuel bundle and a pressure tube. This could produce localised overheating, overstrain and failure of the pressure tube.

iii) If a pressure tube absorbs too much hydrogen at elevated temperatures, it may become embrittled at lower temperatures and fail due to the thermal shock associated with coolant desuperheating and/or channel rewet.

iv) If pressure tube/calandria tube contact is due to pressure tube sag, and if low steam flows and the resultant high fuel temperatures persist, then the top portion of a pressure tube could melt (7). The potential for absorbed oxygen to strengthen the pressure tube or raise its melting point should be assessed.

v) After complete pressure tube/calandria tube contact occurs due to pressure tube ballooning, extensive calandria tube dryout could result in continued channel heatup and failure due to local or global overstrain. Presently available analytical tools and experimental data are adequate to determine whether calandria tube dryout will occur if the moderator temperature is known.

vi) After pressure tube/calandria tube contact due to either pressure tube ballooning or sag, any subsequent thermal or mechanical interaction between the fuel and the pressure tube in a region where calandria tube dryout has persisted could result in localised channel heatup and failure due to local overstrain. This failure mechanism is of particular concern in Pickering A where extensive bundle slumping is predicted (2) and where the long term capability of the spray system to cool the exterior of the channels is questionable. In Pickering A the emergency coolant injection system should be shown to be cooling the fuel before calandria tube sprays are required to cool the channel.

The following sections will discuss pressure tube failure scenarios i) to iii) inclusive and how they were assessed in the Bruce A (1) and Pickering A (2) large break LOCA analyses. Pressure tube failure scenarios iv) to vi) inclusive were not considered in as great depth and therefore will not be discussed further.

1. Hydrogen Embrittlement

Hydrogen embrittlement as a potential pressure tube failure mechanism was not examined in the Bruce A and Pickering A large break LOCA analyses.

Recent experimental data from Canada, Germany and Japan (refer to Figure 4) indicates that hydrogen can be absorbed relatively quickly by Zircaloy-4 fuel sheath material at temperatures greater than 800 C if the hydrogen to steam volume ratio in the surrounding environment is high enough (7). Once absorbed by the Zircaloy, hydrogen will have a strong tendency to diffuse to lower temperature regions where it will precipitate as zirconium hydride platelets if the terminal solid solubility limit is exceeded (7). The terminal solid solubility (TSS) decreases rapidly for temperatures less than 400 C (i.e TSS (400 C) = 200 ppm) (7). Thus, if more than 200 ppm of hydrogen is present in the pressure tube material at elevated temperatures and the temperature decreases to below 400 C, hydride platelets will start to form. These platelets can adversely affect the ductility of the pressure tube.

In the case of contact between pressure tube and calandria tube due to pressure tube sag, hydrogen could be absorbed in the downstream portion or in the overheated upper region of the pressure tube. It could then diffuse circumferentially and/or axially to the lower temperature contact region. In the case of contact due to pressure tube ballooning, hydrogen could be absorbed in the overheated downstream portion of the pressure tube and then diffuse back to the lower temperature contact region.

Experimental work is required to investigate the following:

i) the rate at which hydrogen could be absorbed into Zr - 2.5 wt% Nb pressure tubes at elevated temperatures;

ii) the behaviour of hydrogen in the pressure tube; and

iii) the effect of hydrogen on pressure tube ductility under large break LOCA conditions.

Until further experimental work is available, the failure of pressure tubes due to hydrogen embrittlement cannot be ruled out in Bruce A and Pickering A large break LOCAs.

2. Temperature Gradients

In the large break LOCA analyses for Pickering A and Bruce A, analytical assessments of the potential for circumferential temperature gradients in the pressure tubes were not provided. Ontario Hydro concluded on the basis of limited experimental evidence that circumferential temperature gradients would not result in pressure tube failure prior to pressure tube/calandria tube contact due to ballooning. Despite the limited experimental evidence and the absence of analytical support, Ontario Hydro assumed that all the pressure tubes in early heatup channels ballooned to contact without failure. This represents 240 tubes in Bruce A and 98 in Pickering A.

An experimentally verified computer code is now available to predict the effect of circumferential temperature gradients on the deformation behaviour of as-received Zr - 2.5 wt% Nb pressure tubes (6). Analysis and experiment have shown that fairly steep temperature gradients are required to cause pressure tube failure prior to ballooning contact (7). Steeper gradients still are required as the pressure in the channel decreases. Thus, the problem in a large break LOCA analysis is to predict the potential for circumferential temperature gradients, and their behaviour with time. Once this is known, an existing verified computer code can be used to predict the pressure tube deformation behaviour.

Ontario Hydro assumed that, "The only potentially significant temperature gradient in a pressure tube might be caused by bundle slumping prior to pressure tube ballooning." (1). The potential for thermal/mechanical interaction between the fuel and the pressure tube will be discussed in the next section. However, another scenario that could cause large temperature gradients on the pressure tube is the slumping of the pressure tube into contact with the calandria tube before significant ballooning of the pressure tube occurs. The pressure tube would cool down in the contact region (i.e. assuming calandria tube dryout does not occur) and continue to heat up in the non-contact region. In this case, depending on the channel pressure, transverse strain of the upper portion of the pressure tube could continue.

Pressure tube slumping can occur in the temperature range 800-850 C due to local deformation of the pressure tube about the garter springs in combination with garter spring deformation (7).

An analytical assessment of the slump before strain scenario has been carried out. The results of this assessment have shown that, depending on the nature of the channel depressurisation and temperature transients, conditions can be found where initial pressure tube slumping followed by transverse strain to contact is predicted (7). The "slump/strain" scenario can result in 900 C temperature gradients on the pressure tube (7).

Further analytical work is required to establish the range of pressure tube deformation scenarios that could be expected in large break LOCAs in Bruce A and Pickering A. Once the range of deformation scenarios is established then a better assessment of the potential for pressure tube circumferential temperature gradients can be performed. This will allow a more confident estimate to be made of the possibility of pressure tube failure prior to ballooning contact.

3. Fuel/Pressure Tube Interaction

In the large break LOCA analyses for Bruce A and Pickering A, Ontario Hydro assumed the following:

i) in general, bundle slumping will occur after the pressure tube balloons and contacts the calandria tube; and

ii) if bundle slumping occurs before ballooning contact, the fuel to pressure tube heat transfer coefficient is low enough that a large temperature gradient would not develop on the pressure tube.

There is no relevant experimental information available to support either of these assumptions directly (6,7).

In the Bruce A and Pickering A large break LOCA analyses, fuel bundle slumping was assumed to occur if the temperature exceeded 1850 C anywhere in the fuel bundle. Depending on the assumptions made, CHAN-II(MOD3) can predict fuel bundle slumping according to the "1850 C criterion" but prior to pressure tube ballooning contact. As an example, when the emissivity of Zircaloy was reduced from 0.8 to 0.4 (refer to Table 4, case 3) bundle slumping was predicted to occur 8.0 seconds before pressure tube ballooning contact. During that 8.0 seconds a localised hot region on the pressure tube could develop which could cause pressure tube failure prior to uniform ballooning contact.

Further analyses are required to determine:

i) the range of conditions that could result in thermal/mechanical interaction between the fuel and the pressure tube prior to uniform pressure tube ballooning;

ii) the range of conditions that could result in local pressure tube overheating following this fuel/pressure tube interaction; and

iii) the deformation behaviour of a pressure tube experiencing localised overheating and the effect that this deformation may have on the fuel/pressure tube interaction itself.

Experimental work is required to:

i) determine the deformation behaviour of fuel bundles under large break LOCA conditions; and

ii) determine the relative heatup rates of fuel bundles and pressure tubes under large break LOCA conditions.

Until the results of further analytical and experimental work are available, the potential for thermal/mechanical interaction between the fuel and the pressure tube with consequent local overheating and failure of a pressure tube cannot be confidently estimated.

4. Section Closure

The conclusion reached by Ontario Hydro in the large break LOCA analyses for both Bruce A and Pickering A is that "pressure tube integrity is assured".

In view of the concerns raised in the previous sections, this conclusion cannot be supported confidently.

F. HYDROGEN EVOLUTION

The prediction of the timing and extent of hydrogen evolution from a core during a large break LOCA is needed to determine the potential for hydrogen burns or explosions in containment.

Hydrogen source terms were not provided by Ontario Hydro for the Bruce A and Pickering A large break LOCA analyses. In the Ontario Hydro reference case for a 7.5 MW channel in Bruce A, only 23 g of hydrogen was generated over the first 500 seconds of the accident (7). Given that even less hydrogen would be generated in the more numerous lower power channels, it appears that the hydrogen source terms for Bruce A and Pickering A would be quite low.

From the results of the selected CHAN-II(MOD3) sensitivity analyses on a 7.5 MW channel in Bruce A, the hydrogen generated in the first 500 seconds of the accident ranged from 390 to 800 g.

Thus, depending on the assumptions made when determining fuel and pressure tube temperature transients, there could be a wide range in predictions of both the amount and the rate of hydrogen generation, and its release to containment.

G. RECOMMENDATIONS

Recommendations are provided for further experimental work, model development and analytical assessments in the areas of fuel, fission product and pressure tube behaviour. This work is needed to provide better support for accident analyses in large break LOCAs in Bruce A or Pickering A. In each category the items are arranged in order of decreasing priority.

Experiments will be required for the large scale verification of models that are used to predict large break LOCA, fuel and pressure tube behaviour. However, until some of the model development work described in section G.2 is complete and some of the experimental data from requirements 1.1 to 1.10 are available, the detailed planning of such verification experiments is premature.

1. Experimental Work

1.1 The deformation behaviour of CANDU fuel bundles should be investigated at least over the fuel and sheath temperature range 1500-3000 C in order to determine:

i) the timing, the extent and the thermal and mechanical characteristics of fuel element interaction with the pressure tube;

ii) the extent to which steam can access the interior of deformed fuel bundles, over a range of steam flow conditions, for various degrees of pressure tube transverse strain and fuel bundle deformation;

iii) the characteristics of molten zirconium/uranium eutectic or molten UO2 movement within a deformed fuel bundle. An assessment should be made of the potential for, and the characteristics of, thermal and mechanical interactions between molten zirconium/uranium eutectic or molten UO2 and the pressure tube; and

iv) the characteristics of radial heat transfer through deformed fuel bundles and heat transfer to the pressure tube.

Care should be taken to ensure that the design and performance of the experiments is such that bundle deformation behaviour under the most severe large break LOCA conditions is investigated.

1.2 The potential for hydrogen absorption in Zircaloy and Zr-2.5 wt% Nb should be investigated over a range of temperatures, hydrogen-to-steam volume ratios and flow rates. Emphasis should be placed on determining conditions which lead to rapid hydrogen absorption.

1.3 The mechanical behaviour of Zircaloy and Zr-2.5 wt% Nb pressure tubes containing various amounts and distributions of hydrogen should be investigated over a range of temperatures and stress conditions. Emphasis should be placed on determining conditions which lead to pressure tube failure.

1.4 The emissivity of Zircaloy and zirconium dioxide should be measured over a temperature range which is bounded by the melting point of zirconium dioxide.

1.5 The deformation behaviour of pressure tubes under conditions where localised hotspots are present should be investigated. Emphasis should be placed on determining conditions which lead to local pressure tube failure prior to the development of significant (i.e. 10-15%) overall transverse strain.

1.6 The timing and extent of transient activity release during fuel heatup and isothermal hold should be investigated over a range of fuel heatup rates and isothermal hold temperatures for various initial activity distributions. The range of conditions which result in fuel microcracking and the consequent effect of fuel microcracking on the thermal conductivity of the fuel should also be studied.

1.7 The mechanical behaviour of zirconium dioxide layers which experience thermal cycling at elevated temperatures should be investigated. Emphasis should be placed on determining conditions which lead to extensive oxide cracking or oxide spalling.

1.8 The timing and extent of oxidation of the inner surface of the fuel sheath should be investigated over a range of steam flow conditions and of fuel thermal/mechanical conditions (i.e. sheath and fuel temperatures, characteristics of sheath deformation and rupture). Emphasis should be placed on determining conditions which lead to extensive oxidation of the fuel sheath inner surface.

1.9 An investigation should be made of the nature of the circumferential temperature distributions that can develop on a pressure tube due to asymmetric contact with a calandria tube, prior to significant pressure tube ballooning. Emphasis should be placed on determining conditions which lead to local pressure tube failure prior to pressure tube/calandria tube contact due to pressure tube transverse strain.

1.10 The timing and extent of activity release due to the dissolution of UO2 as a result of the Zr/UO2 interaction should be investigated over a range of fuel thermal and mechanical conditions.

2. Model Development

2.1 A model should be developed to predict the rate of hydrogen absorption into zirconium alloy pressure tubes and the behaviour of hydrogen in the pressure tube under conditions of interest to large break LOCA.

2.2 A pressure tube deformation model should be developed to predict the mechanical behaviour of the pressure tube under conditions where circumferential temperature gradients and localised hotspots could exist and garter springs may or may not be present.

2.3 A model should be developed to predict the thermal and mechanical behaviour of a CANDU fuel bundle and the consequent thermal behaviour of the pressure tube at extremely elevated fuel temperatures. The model should at least utilise the experimental information gained from recommendations 1.1, 1.4, 1.7 and 1.8.

2.4 A model should be developed for CANDU fuel to predict transient activity release and activity release due to UO2 dissolution resulting from the Zr/UO2 interaction.

2.5 The models of recommendations 2.1 through 2.3 should eventually be combined to provide an integrated thermal, mechanical and chemical model of a CANDU fuel channel which could be used to predict fuel and fuel channel behaviour under conditions of interest to large break LOCAs.

3. Analytical Assessments

As previously discussed, the fuel and pressure tube temperature transients predicted by the CHAN-II computer codes are extremely sensitive to the input data and assumptions regarding fuel and pressure tube thermal/mechanical behaviour. Care must be taken to ensure that, where uncertainties exist with respect to input data and assumptions, values are chosen such that predicted fuel temperatures are maximised.

The results of the following assessments will provide information which will help in the definition of some of the experimental work recommended in section G.1:

3.1 CHAN-II calculations should be performed to determine more clearly the effect of input data and parameter uncertainties on predicted fuel and pressure tube temperatures. Some of the input data and parameters that should be investigated include:

i) the bundle slumping temperature;

ii) the contact angle for bundle slumping;

iii) the pressure tube/calandria tube contact conductance;

iv) the fuel bundle/pressure tube contact conductance;

v) the fuel thermal conductivity;

vi) the emissivities of the fuel sheaths and pressure tube;

vii) the fuel-to-sheath heat transfer coefficient;

viii) the inlet steam flow;

ix) the inlet steam temperature;

x) the potential for double-sided sheath oxidation;

xi) the potential for more rapid oxidation rates at temperatures greater than 1500 C;

xii) the potential for hydrogen absorption in the fuel sheath and/or pressure tube;

xiii) the initial fuel temperature distribution;

xiv) the time after initiation of the transient that the CHAN-II calculation is started (i.e. controls fuel decay power level);

xv) the timing and extent of pressure tube transverse strain; and

xvi) the flow distribution in the channel as a function of pressure tube and bundle deformation.

The sensitivity studies should be performed with a modified version of the CHAN-II code in which all of Ontario Hydro's assumptions with respect to "turning off" the exothermic Zircaloy/steam reaction and convective heat transfer have been removed and the error in the calculation of the centre pin fuel temperature has been corrected.

3.2 Further sensitivity studies should be performed to provide a better estimate of the potential for local pressure tube overheating due to thermal and mechanical interaction between fuel elements and the pressure tube under conditions of interest to large break LOCAs.

3.3 Further calculations should be performed to estimate the thermal and mechanical conditions that will lead to pressure tube failure, prior to uniform pressure tube/calandria tube contact due to ballooning, under conditions of interest to large break LOCAs.

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The authors assume no liability with respect to any damage of loss incurred as a result of the use made of the information contained in this publication.

Table 1

Times (Seconds) at Which Pressure Tube/Calandria Tube Contact due to Pressure Tube Ballooning is Predicted to Occur for Early Heatup Channels in Bruce A and Pickering A LOCA Analyses (1,2)

CHANNEL POWER(MW)		AXIAL BUNDLE POSITION								
Bruce A	Pickering A	3	4	5	6	7	8	9	10	11
7.5		--	--	26	16	14	15	19	27	60
	6.0	28	18	16	14	14	14	15	17	25
6.7		--	--	39	23	19	19	24	35	--
	5.3	37	22	18	16	15	16	17	19	29
6.2		--	--	--	30	24	24	30	--	83
	4.9	50	25	20	18	17	17	18	21	31
5.7		--	--	--	45	31	29	38	--	--
	4.5	--	32	24	20	19	19	21	25	44
4.6		--	--	--	--	--	66	76	--	--
	3.7	--	--	51	37	32	32	33	39	--

Table 2

Times (Seconds) at Which Bundle Slumping is Predicted to Occur for Early Heatup Channels in Bruce A and Pickering A LOCA Analyses (1,2)

CHANNEL POWER(MW)		AXIAL BUNDLE POSITION							
Bruce A	Pickering A	3	4	5	6	7	8	9	10
7.5		--	--	163	95	79	90	158	354
	6.0	165	57	34	25	22	24	30	52
6.7		--	--	260	148	133	144	226	--
	5.3	--	101	50	35	31	34	44	97
6.2		--	--	--	244	202	223	--	--
	4.9	--	193	149	103	86	86	96	145
5.7		--	--	--	--	324	411	--	--
	4.5	--	--	201	152	139	156	--	--
4.6		--	--	--	--	--	--	--	--
	3.7	--	--	--	--	--	--	--	--

Table 3

Throughwall Oxidation Times (in Seconds)
-Fuel Sheath-
(Based on Oxidation Rates from Urbanic-Heidrick)

Temperature	Oxidation Kinetics			
	Parabolic		Linear	
	Single	Double	Single	Double
1273	1.4(5)*	3.6(4)	378.	189.
1373	6.6(4)	1.6(4)	256.	128.
1473	3.4(4)	8.4(3)	183.	92.
1573	1.9(4)	4.7(3)	137.	69.
1673	1.1(4)	2.8(3)	106.	53.
1773	7.0(3)	1.8(3)	84.	42.
1873	1.1(3)	2.7(2)	33.	17.
1973	6.9(2)	1.7(2)	26.	13.
2073	4.7(2)	1.2(2)	21.	11.

*$1.4(5) = 1.4 \times 10^{5}$

Single - single-sided oxidation attack

Double - double-sided oxidation attack

Table 4

Maximum Fuel Temperature from CHAN-II(MOD3)
Predictions for a 7.5 MW Channel in Bruce A

	Maximum Fuel Temperature (C)	Change in Fuel Temperature (C)
1. OH Reference	2344	- 639
2. Reference case- this work (7)	2983	0
3. Case 2 + reduced Zircaloy emissivities	3119	+ 136
4. Case 2 + reduced fuel thermal conductivity	3170	+ 187
5. Case 2 + double sided oxidation	3136	+ 153
6. Case 2 + pressure tube sag not ballooning	3263	+ 280
7. Case 2 + all previous modifications	3578	+ 595
8. Case 7 with 100g/s flow	2750	- 233

(1) Change in maximum fuel temperature determined in reference to case 2.

Table 5

Components of Half Core Activity Release for Bruce A "Early Heatup" Channel Temperatures (1)

Release Component (MCi)	Fuel Heatup Rate (C/s)	
	1	5
Free Inventory (Half Core)		
- all species*	9.6	9.6
- I-131	1.34	1.34
FASTGRASS Predicted Transient Release (During Ramp)		
- all species	37.1	22.7
- I-131	1.1	0.7
Zr/UO2 Interaction (T > 1750C)		
- all species	2.0	2.0
- I-131	0.07	0.07
Total		
- all species	48.7	34.3
- I-131	2.51	2.11

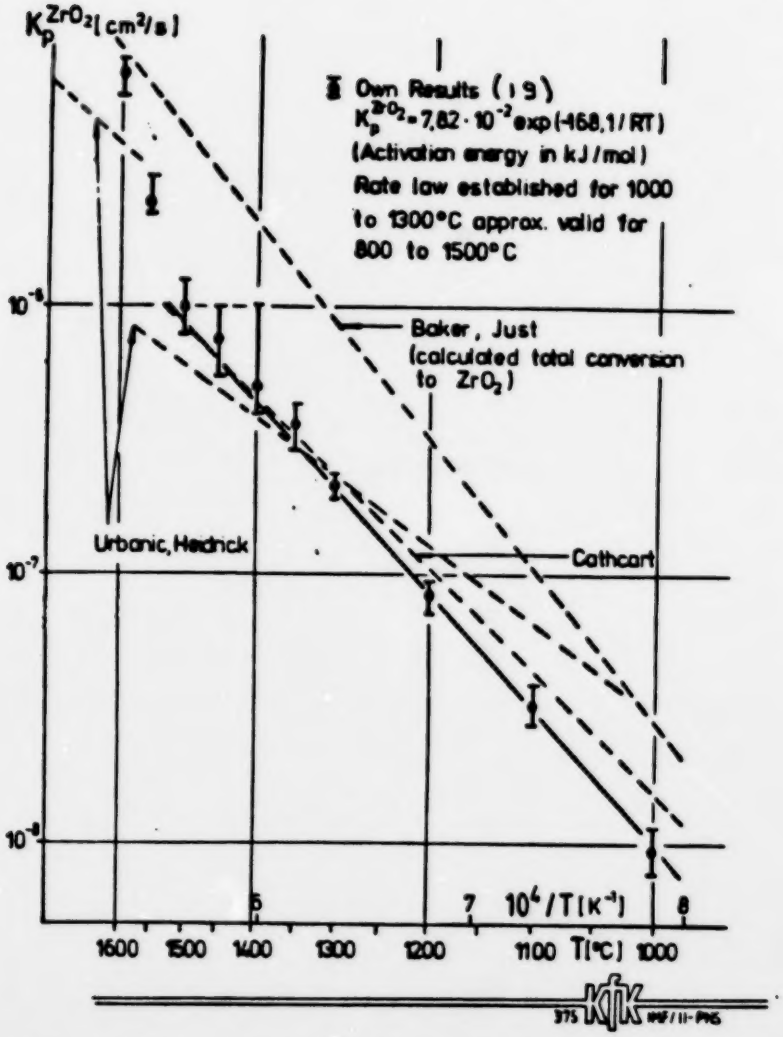
* all species with half lives greater than 3 minutes

Table 6

Components of Half Core Activity Release for Bruce A Using 600 MW LOCA/LOECI Channel Temperatures (17)

Release Component (MCi)	Fuel Heatup Rate (C/s)	
	1	5
Free Inventory (Half Core)		
- all species*	9.6	9.6
- I-131	1.34	1.34
FASTGRASS Predicted Transient Release (During Ramp)		
- all species	156.0	89.0
- I-131	4.4	2.5
Zr/UO2 Interaction (T > 1750C)		
- all species	10.1	10.1
- I-131	0.35	0.35
Total		
- all species	175.7	108.7
- I-131	6.1	4.2

* all species with half lives greater than 3 minutes



Arrhenius Representation of Parabolic Rate of ZrO_2 Scale Growth during Zircaloy-4 / Steam HT Oxidation

Figure 1
Zircaloy-4 Oxidation Data
Leistikow et al (19)

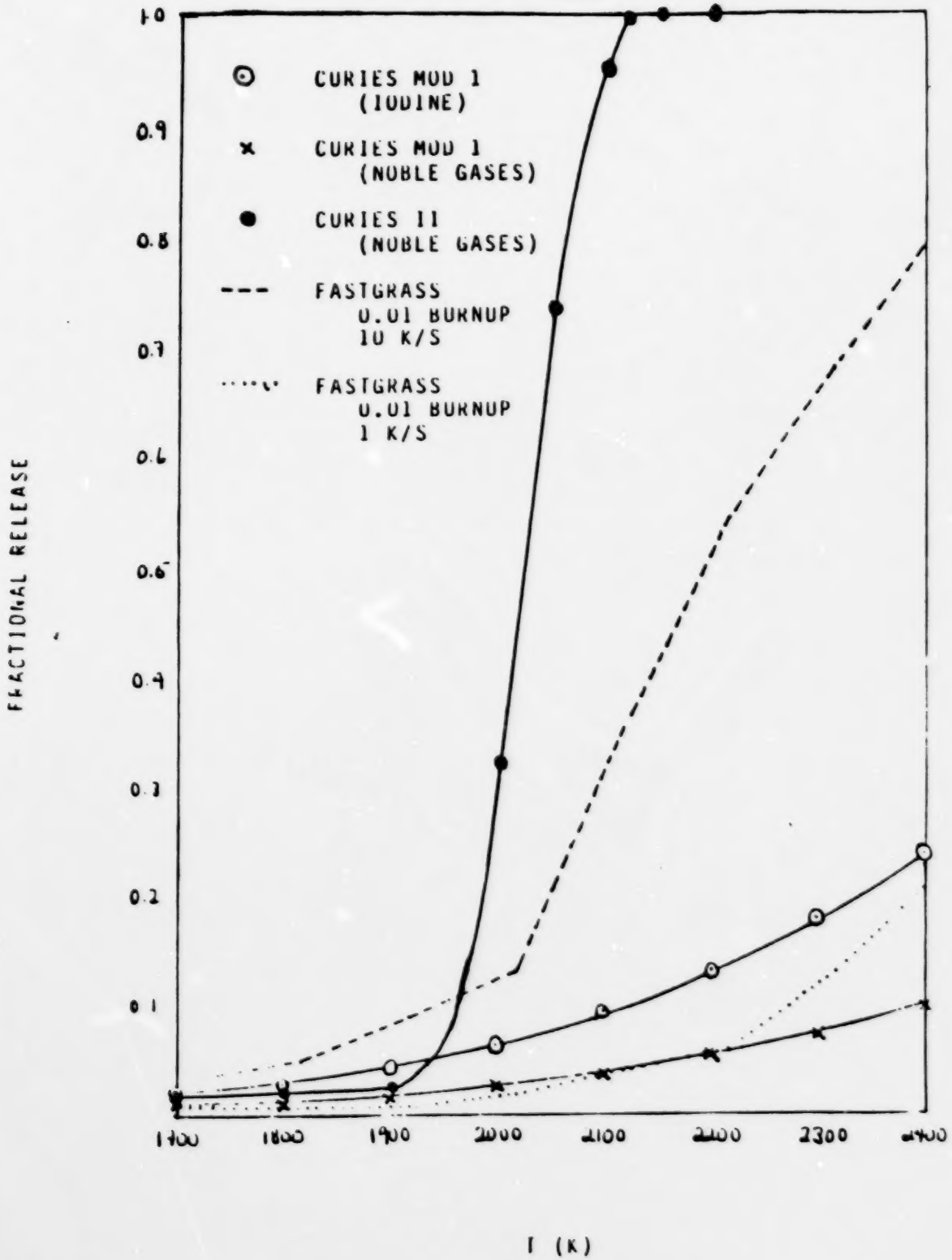


Figure 2. Release predictions of CURIES MOD 1, CURIES II (200 s hold at temperature) and FASTGRASS (temperature ramp, no hold).

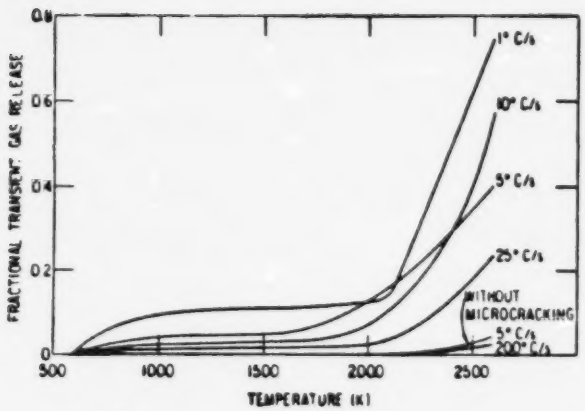


Figure 3
Transient Gas Release Fractions
-FASTGRASS Predictions-
As-irradiated Temperature = 1200K
Grain Size = 10 microns
Burnup = 0.1 atomic %

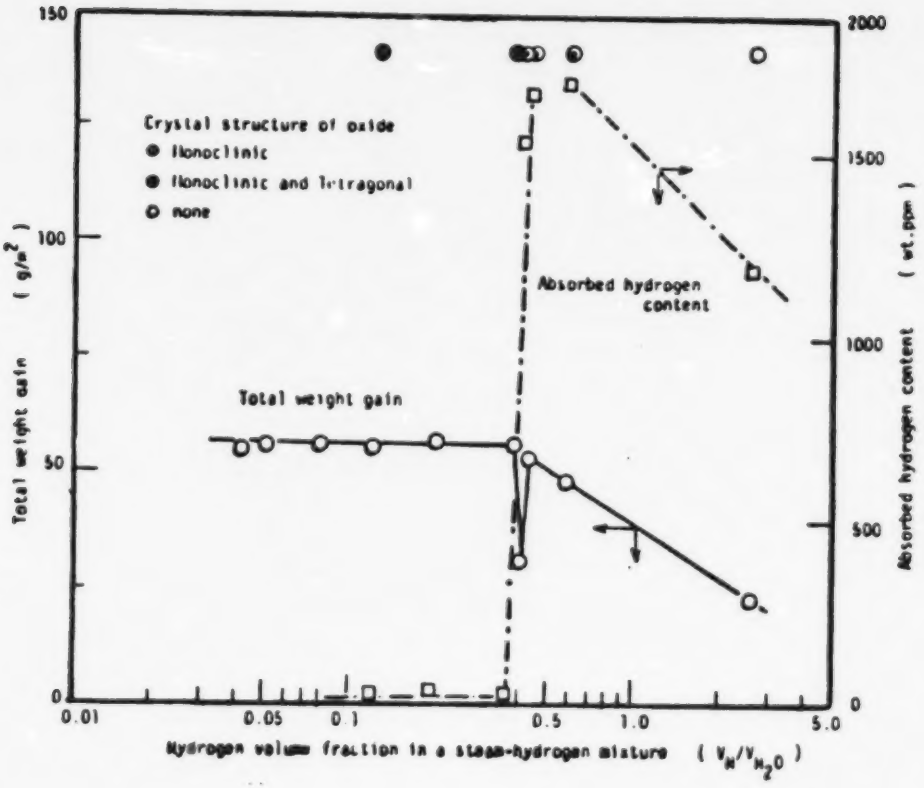


Figure 4
Effect of Hydrogen Volume Fraction on Oxidation Behaviour of Specimens Oxidized at 1273K for 600s in a Steam-Hydrogen Mixture (7)